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Syntheses, crystal structure and thermal behavior of poly[di-μ-bromido-μ-2,3-dimethylpyrazine-$\kappa^2N^1{:}N^4$-cadmium(II)]

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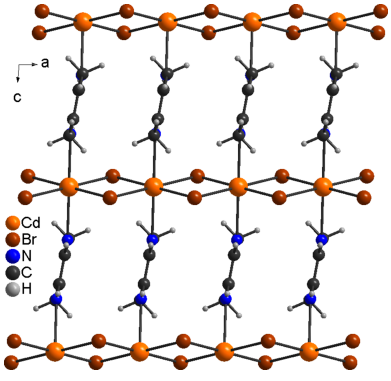
The title compound, $[CdBr_2(C_6H_8N_2)]_n$, was prepared by the reaction of cadmium bromide with 2,3-dimethylpyrazine in acetonitrile. Powder X-ray diffraction (PXRD) indicated that a pure phase had been obtained. The asymmetric unit consists of one Cd cation located on a center of inversion, one 2,3-dimethylpyrazine ligand situated on a twofold rotation axis and one bromide anion in a general position. In the extended structure, the cadmium cation is octahedrally coordinated by four bridging bromide anions and two bridging 2,3-dimethylpyrazine coligands. The cations are linked *via* common bromide-ion edges into [010] chains that are further connected into (100) layers by the bridging 2,3-dimethylpyrazine coligands. Measurements using thermogravimetry and differential thermoanalysis reveal that the compound decomposes in two separate steps in which a more 2,3-dimethylpyrazine-deficient compound is formed, which according to PXRD measurements is crystalline.

1. Chemical context

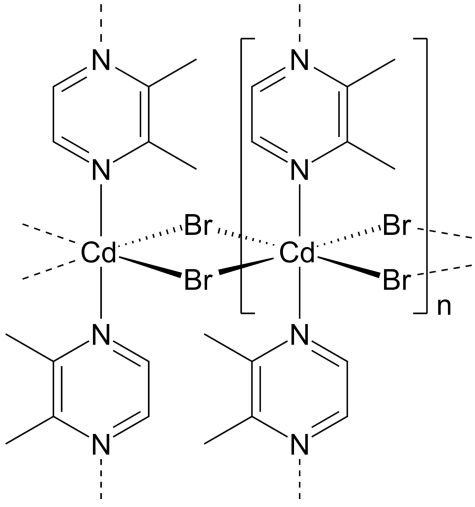
For many years, we and others have been interested in the crystal structures of transition-metal halide and pseudohalide coordination compounds because they show a large structural variability, which frequently leads to the formation of different metal halide substructures (Kromp & Sheldrick, 1999; Peng *et al.*, 2010; Li *et al.*, 2005; Näther *et al.*, 2002). In the beginning, we focused on compounds with copper(I) halides and pseudohalides and later this was expanded to divalent cations like zinc or cadmium. What is common to all of these compounds is the fact that for a given metal halide and a given coligand, in most cases compounds of different stoichiometry can be obtained. If this is the case, the coligand-deficient compounds can frequently be detected and prepared by thermal ligand removal, because the coligands are usually lost in separate steps (Näther *et al.*, 2001; Näther & Jess, 2001).

In the course of our project we became interested in zinc and cadmium halide coordination compounds with 2,3-dimethylpyrazine ($C_6H_8N_2$) as coligand. With CdI_2 a coligand-rich compound with the composition $CdI_2(C_6H_8N_2)_2$ and a coligand-deficient compound with the composition $CdI_2(C_6H_8N_2)$ were obtained (Näther, 2026*a*). The first compound consists of discrete complexes with cadmium in a tetrahedral environment. In the second compound, the cadmium cations are also tetrahedrally coordinated and linked by the 2,3-dimethylpyrazine ligands into chains. These structures are therefore very similar to those of the corresponding compounds with zinc halides (Näther & Bhosekar, 2025*a*,*b*, 2026; Yang *et al.*, 2025). These structures with CdI_2 are somehow surprising because, in contrast to zinc, an octahedral



coordination is usually preferred for cadmium halide coordination compounds. Therefore, for these compounds structures were expected in which the Cd cations are linked by pairs of iodide anions into chains. In this case, the 2,3-dimethylpyrazine coligand would be terminally coordinated in $CdI_2(C_6H_8N_2)_2$, whereas in $CdI_2(C_6H_8N_2)$ the coligand would act as a bridging ligand. This is exactly the case for the corresponding compounds with, for example, pyrazine, 2-methylpyrazine and 2-chloropyrazine as coligand (Bailey & Pennington, 1997; Pickardt & Staub, 1997; Näther *et al.*, 2017).

Based on these findings, we tried to prepare the corresponding compounds with cadmium bromide and we accidentally obtained crystals of a solvate with the composition $CdBr_2(C_6H_8N_2)(H_2O)\cdot C_6H_8N_2\cdot 0.5H_2O$, in which the ratio between $CdBr_2$ and coordinating coligands is 1:2 (Näther, 2026*b*). In contrast to the corresponding compounds with CdI_2, in this structure $CdBr_2$ chains occur and an octahedral coordination of the cadmium cations is observed. Therefore, one can assume that a more coligand-deficient compound with the composition $CdBr_2(C_6H_8N_2)$ might exist, in which similar $CdBr_2$ chains are connected by the 2,3-dimethylpyrazine ligands into layers. To investigate this assumption, additional synthetic investigations were performed in which crystals of the title compound were obtained, which were characterized by single crystal X-ray diffraction.



2. Structural commentary

The asymmetric unit of the title compound, $CdBr_2(C_6H_8N_2)$ ($C_6H_8N_2$ = 2,3-dimethylpyrazine) (**I**) (Fig. 1), is built up from one cadmium cation that occupies a center of inversion, one 2,3-dimethylpyrazine ligand generated by a twofold rotation axis bisecting the pairs of ring carbon atoms, and one bromide anion in a general position. Crystal symmetry leads to the cadmium cations being sixfold coordinated by four bromide anions that are located in the basal plane and two 2,3-dimethylpyrazine ligands in the apical positions. Bond angles deviate from the ideal values (Table 1), which shows that the Cd cation is in a slightly distorted octahedral environment (Table 1). The cations are linked by pairs of μ-1,3 bridging bromide anions into linear chains that propagate in the crystallographic *b*-axis direction (Fig. 2). These chains are built up from octahedra that share common bromide-ion edges [Br···Br = 3.760 (2) Å]. The bridging co-ligands connect the chains into (100) layers.

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.531 (4)	Cd1—Br1^{i}	2.7741 (5)
Cd1—Br1	2.6789 (5)		
N1—Cd1—Br1^{ii}	91.66 (10)	N1^{ii}—Cd1—Br1^{i}	94.08 (10)
N1—Cd1—Br1	88.34 (10)	Br1^{ii}—Cd1—Br1^{i}	87.157 (14)
N1—Cd1—Br1^{i}	85.92 (10)	Br1—Cd1—Br1^{i}	92.843 (14)

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y+1, -z+1$.

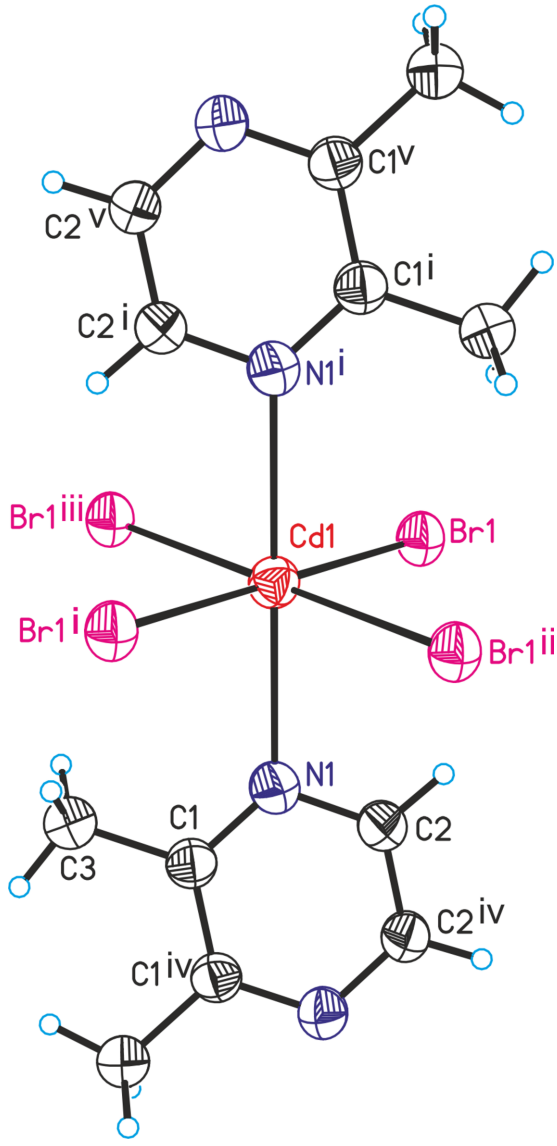


Figure 1
The asymmetric unit of (**I**) expanded to show the complete ligands and cadmium coordination polyhedron with displacement ellipsoids drawn at the 50% probability level. Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+1, y, z$; (iii) $-x, -y+1, -z+1$; (iv) $-x+1, y, -z+\frac{1}{2}$; (v) $x, y+1, z+\frac{1}{2}$.

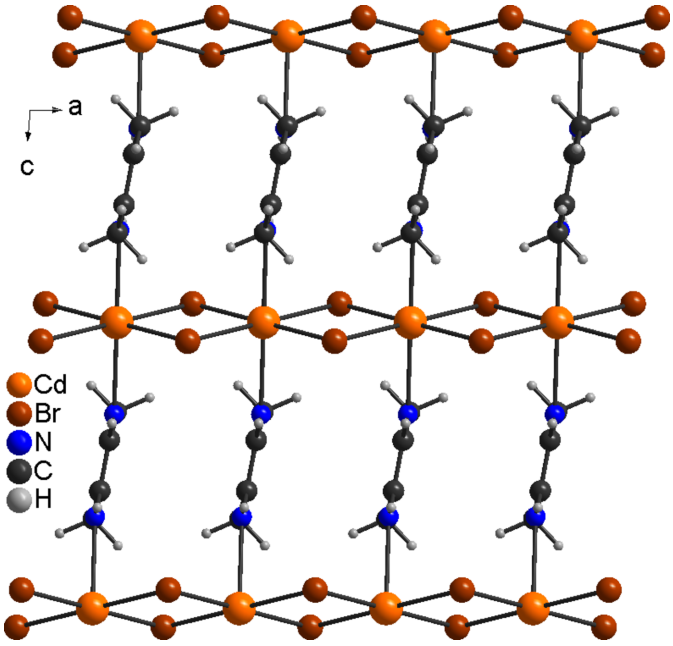


Figure 2
View of a part of a chain in the crystal structure of (**I**).

This structure is therefore completely different from that of $CdI_2(C_6H_8N_2)$ (Näther, 2026*a*) in which the cadmium cations are in a tetrahedral environment, which might be more stable because of repulsion between the bulky iodide anions. However, there are a number of compounds with other pyrazine derivatives reported that show the same topology of the coordination network as that in the title compound. This also includes compounds with CdI_2, which shows that the situation is more complex. With pyrazine as ligand this includes CdX_2(pyrazine) (X = Cl, Br, I; CSD refcodes TISSUJ, RINSIQ, RINSOW, Bailey & Pennington, 1997; RINSOW01, Pickardt & Staub, 1997; RINSOW02, Niu *et al.*, 2005). This also includes compounds with 2-methylpyrazine as ligand such as the isotypic compounds CdX_2(2-methylpyrazine) (X = Cl, Br, QAWHEE and QAWHUU, Näther *et al.*, 2017) and CdI_2(2-methylpyrazine) (QAWHAA, Näther *et al.*, 2017).

3. Supramolecular features

In the extended structure of (**I**), the layers are stacked perpendicular to the crystallographic *a*-axis direction (Fig. 3). There are two C—H···Br contacts with one of them at a long distance (H···Br = 3.03 Å) and an angle far from linearity, indicating a very weak interaction. The second one between a methyl hydrogen atom and the bromide atom is shorter with an angle close to linearity, indicating a stronger interaction (Table 2).

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···Br1	0.95	3.03	3.604 (5)	120
C3—H3B···Br1^{iii}	0.98	2.80	3.739 (6)	162

Symmetry code: (iii) $-x, -y+1, -z+1$.

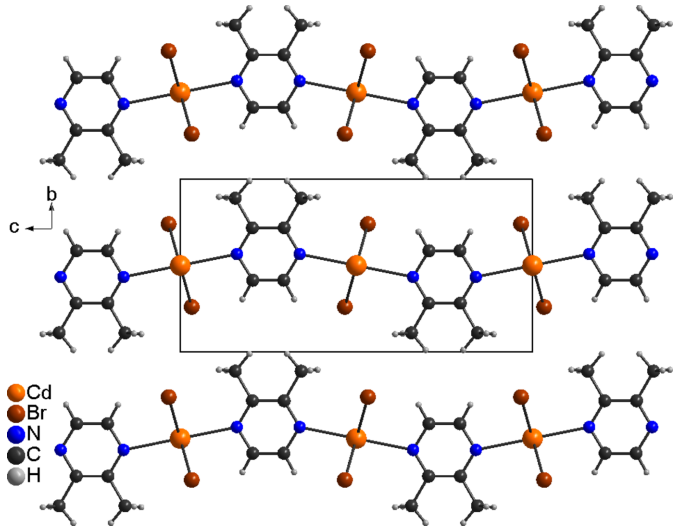


Figure 3
Crystal structure of (**I**) with view along the crystallographic *a*-axis direction.

4. Additional characterization

Comparison of the experimental X-ray powder pattern of (**I**) with that calculated from single-crystal data shows that the title compound has been obtained as a pure phase (Fig. 4). Measurements using thermogravimetry coupled to differential thermoanalysis show that the title compound decomposes in two separate and endothermic steps, in which a 2,3-dimethylpyrazine deficient compound is formed as an intermediate (Fig. 5). PXRD data show that this intermediate is of

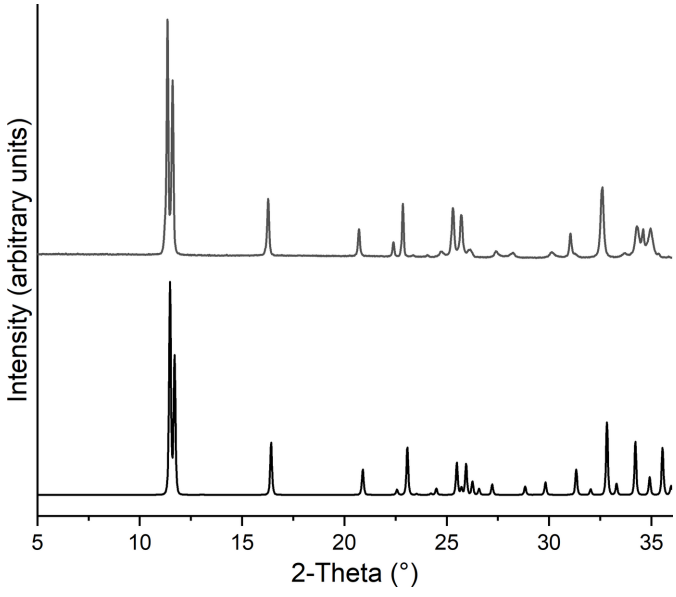


Figure 4
Experimental (top) and calculated (bottom) powder patterns for the title compound.

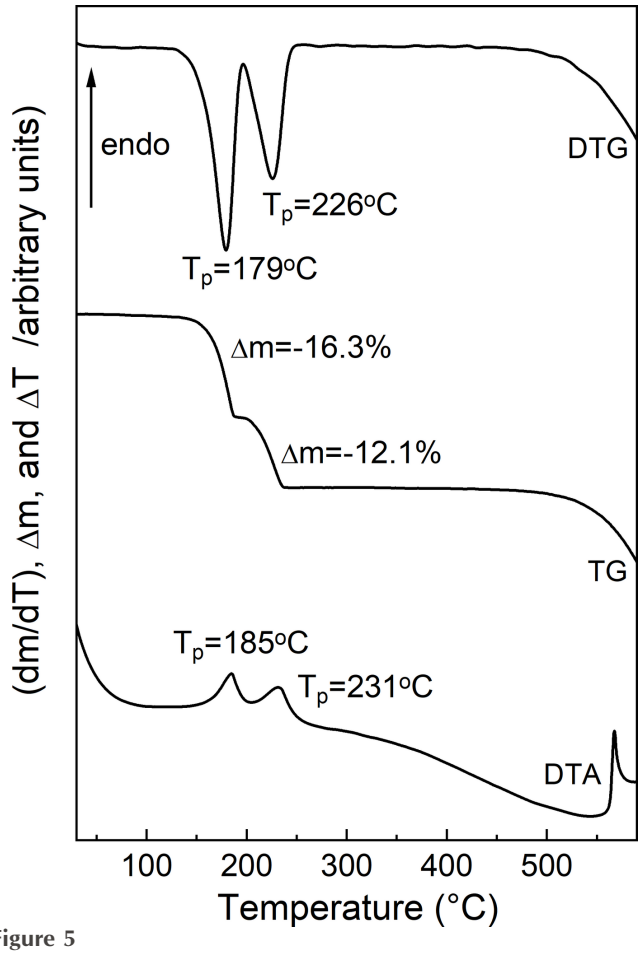


Figure 5
DTG, TG and DTA curves for the title compound.

reasonable crystallinity (Fig. 6). However, the experimental mass loss is not in good agreement with that calculated for the removal of half of the 2,3-dimethylpyrazine ligands and therefore, conclusions concerning the composition of this new crystalline phase cannot be made. In this context it is noted that compounds are reported that exhibit an unusual ratio between the cadmium halide and the organic coligands as in *catena*[hexakis(μ_3-chloro)tetrakis(μ_2-chloro)bis[μ_2-1,2-bis-(1*H*-benzotriazol-1-yl)ethane]pentacadmium]] with a ratio of 2:5 (EMOWAF, Zhai *et al.*, 2011). In any case this intermediate compound must have a more condensed CdI_2 network with μ_3-bridging bromide anions.

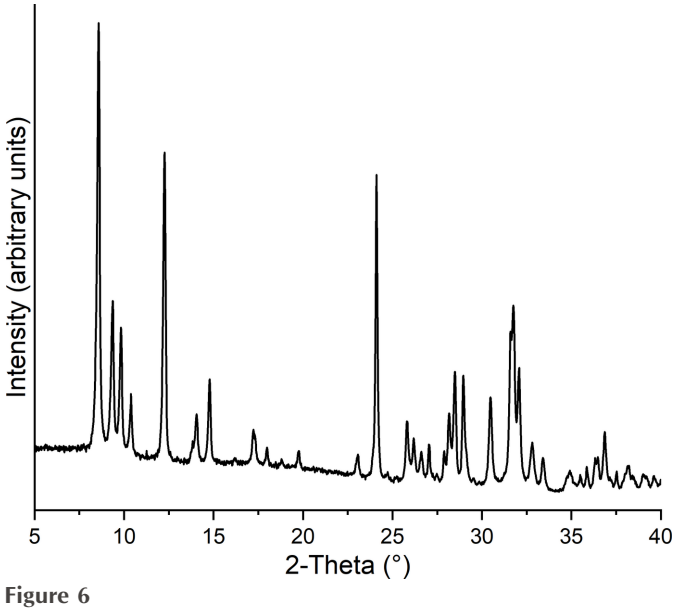


Figure 6
Experimental powder pattern of the residue obtained after the first mass loss in a TG measurement of the title compound.

5. Database survey

As already mentioned in the *Chemical context* section, some compounds with zinc halides and 2,3-dimethylpyrazine are known, and in all of them the zinc cations are tetrahedrally coordinated. This coordination is also found in the cadmium iodide coordination compounds with 2,3-dimethylpyrazine as coligand whereas in the only known compound with CuBr, an octahedral coordination and CuBr chains are observed and this was the origin of the present work.

It was also mentioned that many compounds with other pyrazine derivatives and cadmium halide chains found in the Cambridge Structural Database (CSD Version 5.43, 2025; Groom *et al.*, 2016) using CONQUEST (Bruno *et al.*, 2002) are built up of CdX_2 chains, indicating that an octahedral coordination is preferred. That the situation is more complex is obvious from a search for CdX_2 compounds with similar but monocoordinating ligands, and pyridine and its derivatives would be representative examples. With pyridine, many compounds with cadmium halides are reported in which the ratio between CdX_2 and pyridine is 1:2. For such compounds, both a tetrahedral and an octahedral coordination is found. $CdCl_2$(pyridine)$_2$ consists of $CdCl_2$ chains with octahedral cadmium cations (CDPYCL01; Paulus, 1969, CDPYCL03; Satoh *et al.*, 2001 and CDPYCL04; Hu *et al.*, 2003). The same structure is found for $CdBr_2$(pyridine)$_2$, which crystallizes in two different polymorphic modifications (Hu *et al.*, 2003). In contrast, for CdI_2(pyridine)$_2$, discrete complexes with a tetrahedral coordination of the Cd cations are observed (IPPAYAZ01; Hu *et al.*, 2003). Similar structures are found with 3-methylpyridine. $CdCl_2$(3-methylpyridine)$_2$ (BASQOC; Satoh *et al.*, 2001 and BASQOC01; Hu *et al.*, 2003) and $CdBr_2$(3-methylpyridine)$_2$ (IPAZOO, Hu *et al.*, 2003) show the same chain structure, while CdI_2(3-methylpyridine)$_2$ (IPEBAG; Hu *et al.*, 2003) consists of discrete tetrahedral complexes. Finally, the corresponding compounds with 2-methylpyridine, $CdBr_2$(2-methylpyridine)$_2$ (EYEROQ; Bowmaker *et al.*, 2011) and CdI_2(2-methylpyridine)$_2$ (EYESOR; Bowmaker *et al.*, 2011), crystallize as discrete complexes, while the structure of the chloride compound is unknown. For the latter compounds, this might be traced back to steric repulsion between the metal cations and the methyl group in an octahedral coordination. This also suggests that for the iodide compound with pyridine derivatives, the formation of discrete complexes originates from steric reasons because of the much larger radii of iodide anions but it must

be kept in mind that in CdI_2(pyrazine) (RINSOW; Bailey & Pennington, 1997), a chain structure is found.

6. Synthesis, crystallization and experimental details

Cadmium bromide and 2,3-dimethylpyrazine were purchased from Sigma-Aldrich: 0.5 mmol (136.1 mg) $CdBr_2$ and 0.5 mmol (54.1 mg) 2,3-dimethylpyrazine were stirred in 2 ml of acetonitrile for 2 d at room-temperature. Without stirring, single crystals of (**I**) in the form of colorless blocks were obtained within 3d.

The PXRD measurements were performed with Cu $K\alpha_1$ radiation (λ = 1.540598 Å) using a Stoe Transmission Powder Diffraction System (STADI P) equipped with a MYTHEN 1K detector and a Johansson-type Ge(111) monochromator.

Thermogravimetry and differential thermoanalysis (TG-DTA) measurements were performed in a dynamic air atmosphere in Al_2O_3 crucibles using a STA-PT 1000 thermobalance from Linseis. The instrument was calibrated using standard reference materials.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The hydrogen atoms were positioned with idealized geometry (methyl H atoms allowed to rotate but not to tip) and were refined as riding atoms with U_{iso}(H) = 1.2 U_{eq}(C) (1.5 for methyl H atoms). The crystal chosen for data collection was found to be twinned. Both domains were indexed separately and finally a twin refinement using data in HKLF-5 format was performed leading to an BASF parameter of 0.212 (4).

Table 3
Experimental details.

Crystal data	
Chemical formula	$[CdBr_2(C_6H_8N_2)]$
M_r	380.36
Crystal system, space group	Monoclinic, *P*2/*c*
Temperature (K)	170
a, *b*, *c* (Å)	3.9508 (2), 7.5573 (4), 15.4616 (9)
β (°)	94.841 (5)
V (Å^3)	460.00 (4)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	11.00
Crystal size (mm)	0.14 × 0.10 × 0.08
Data collection	
Diffractometer	IPDS2
Absorption correction	Numerical (*X-RED* and *X-SHAPE*; Stoe, 2002)
T_{min}, T_{max}	0.124, 0.286
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	905, 905, 816
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.616
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.034, 0.089, 1.09
No. of reflections	905
No. of parameters	54
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.02, −0.79

Computer programs: *X-AREA* (Stoe, 2008), *SHELXT2014/4* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg, 1999), *XP* in *SHELXTL-PC* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

Acknowledgements

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supporting information

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Syntheses, crystal structure and thermal behavior of poly[di-μ-bromido-μ-2,3-dimethylpyrazine-κ^2N^1:N^4-cadmium(II)]

Christian Näther

Computing details

Poly[di-μ-bromido-μ-2,3-dimethylpyrazine-κ^2N^1:N^4-cadmium(II)]

Crystal data

$[CdBr_2(C_6H_8N_2)]$
M_r = 380.36
Monoclinic, $P2/c$
a = 3.9508 (2) Å
b = 7.5573 (4) Å
c = 15.4616 (9) Å
β = 94.841 (5)°
V = 460.00 (4) Å^3
Z = 2
$F(000)$ = 352
D_x = 2.746 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8176 reflections
θ = 1.3–26.7°
μ = 11.00 mm^{-1}
T = 170 K
Block, colorless
0.14 × 0.10 × 0.08 mm

Data collection

IPDS-2 diffractometer
ω scans
Absorption correction: numerical (X-Red and X-Shape; Stoe, 2002)
T_{min} = 0.124, T_{max} = 0.286
905 measured reflections
905 independent reflections
816 reflections with $I > 2\sigma(I)$
θ_{max} = 26.0°, θ_{min} = 2.6°
h = −4→4
k = −9→9
l = −1→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.089
S = 1.09
905 reflections
54 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0624P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.02 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refined as a 2-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.500000	0.500000	0.500000	0.0371 (2)
Br1	0.00584 (12)	0.73950 (6)	0.46734 (4)	0.0399 (2)
N1	0.4662 (12)	0.4338 (5)	0.3390 (3)	0.0404 (9)
C1	0.4814 (13)	0.2822 (6)	0.2952 (4)	0.0367 (10)
C2	0.4840 (13)	0.5847 (6)	0.2938 (3)	0.0400 (12)
H2	0.474305	0.694575	0.323386	0.048*
C3	0.4525 (16)	0.1113 (7)	0.3437 (4)	0.0443 (11)
H3A	0.287711	0.033896	0.311400	0.066*
H3B	0.376217	0.135673	0.401232	0.066*
H3C	0.674531	0.052770	0.350202	0.066*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0374 (3)	0.0367 (3)	0.0372 (3)	0.00148 (18)	0.0033 (2)	0.00196 (18)
Br1	0.0384 (3)	0.0354 (3)	0.0460 (4)	0.00116 (19)	0.0042 (3)	0.0029 (2)
N1	0.044 (2)	0.036 (2)	0.041 (2)	0.0024 (18)	0.0038 (19)	−0.0008 (18)
C1	0.035 (2)	0.037 (2)	0.038 (3)	0.0003 (19)	0.0058 (19)	0.001 (2)
C2	0.049 (3)	0.036 (3)	0.035 (3)	0.000 (2)	0.002 (2)	−0.001 (2)
C3	0.053 (3)	0.040 (3)	0.040 (3)	−0.001 (2)	0.009 (3)	0.000 (2)

Geometric parameters (Å, º)

Cd1—N1	2.531 (4)	C1—C1^{iv}	1.418 (11)
Cd1—N1^{i}	2.531 (4)	C1—C3	1.503 (7)
Cd1—Br1^{i}	2.6789 (5)	C2—C2^{iv}	1.372 (10)
Cd1—Br1	2.6789 (5)	C2—H2	0.9500
Cd1—Br1^{ii}	2.7741 (5)	C3—H3A	0.9800
Cd1—Br1^{iii}	2.7741 (5)	C3—H3B	0.9800
N1—C1	1.335 (6)	C3—H3C	0.9800
N1—C2	1.342 (6)		
N1—Cd1—N1^{i}	180.00 (4)	C1—N1—C2	117.3 (5)
N1—Cd1—Br1^{i}	91.66 (10)	C1—N1—Cd1	131.9 (3)
N1^{i}—Cd1—Br1^{i}	88.33 (10)	C2—N1—Cd1	110.1 (3)
N1—Cd1—Br1	88.34 (10)	N1—C1—C1^{iv}	120.9 (3)
N1^{i}—Cd1—Br1	91.66 (10)	N1—C1—C3	118.4 (5)
Br1^{i}—Cd1—Br1	180.0	C1^{iv}—C1—C3	120.7 (3)
N1—Cd1—Br1^{ii}	85.92 (10)	N1—C2—C2^{iv}	121.8 (3)
N1^{i}—Cd1—Br1^{ii}	94.08 (10)	N1—C2—H2	119.1
Br1^{i}—Cd1—Br1^{ii}	87.157 (14)	C2^{iv}—C2—H2	119.1
Br1—Cd1—Br1^{ii}	92.843 (14)	C1—C3—H3A	109.5
N1—Cd1—Br1^{iii}	94.08 (10)	C1—C3—H3B	109.5
N1^{i}—Cd1—Br1^{iii}	85.92 (10)	H3A—C3—H3B	109.5
Br1^{i}—Cd1—Br1^{iii}	92.843 (14)	C1—C3—H3C	109.5

Br1—Cd1—Br1^{iii}	87.157 (14)	H3A—C3—H3C	109.5
Br1^{ii}—Cd1—Br1^{iii}	180.0	H3B—C3—H3C	109.5
Cd1—Br1—Cd1^{v}	92.843 (14)		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*+1, *y*, *z*; (iii) −*x*, −*y*+1, −*z*+1; (iv) −*x*+1, *y*, −*z*+1/2; (v) *x*−1, *y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Br1	0.95	3.03	3.604 (5)	120
C3—H3*B*···Br1^{iii}	0.98	2.80	3.739 (6)	162

Symmetry code: (iii) −*x*, −*y*+1, −*z*+1.